

Isovector proton-neutron pairing and Wigner energy in Hartree-Fock mean field calculations

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Abstract

We propose a new approach for the treatment of isovector pairing in self-consistent mean field calculations which conserves exactly the isospin and the particle number in the pairing channel. The mean field is generated by a Skyrme-HF functional while the isovector pairing correlations are described in terms of quartets formed by two neutrons and two protons coupled to the total isospin $T=0$. In this framework we analyse the contribution of isovector pairing to the symmetry and Wigner energies. It is shown that the isovector pairing provides a good description of the Wigner energy, which is not the case for the mean field calculations in which the isovector pairing is treated by BCS-like models.

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In the last years a lot of effort has been dedicated to the understanding of the role played by the proton-neutron pairing in the binding energies of nuclei with $N \approx Z$. The experimental masses indicate that the nuclei with $N = Z$ have an additional binding compared to the neighbouring nuclei. In the phenomenological mass formulas [1] this additional binding energy is taken into account through a term proportional to $|N - Z|$, called usually the Wigner energy. In the extensive mean-field calculations of nuclear masses the Wigner energy cannot be accounted for and therefore it is added as an *ad hoc* phenomenological term [2].

There is a long debate about the origin of the Wigner energy (e.g., see [3] and references quoted therein). In some studies it is supposed that the Wigner energy originates from the proton-neutron pairing correlations, which become stronger in $N=Z$ nuclei. Thus, it was recently argued that the isovector proton-neutron pairing can describe most of the extra binding associated to the Wigner energy, provided the isovector pairing is treated beyond the BCS approximation [4, 5].

The fact that BCS-like models are not appropriate for calculating the contribution of the isovector pairing correlations to Wigner energy can be clearly seen when they are applied for a degenerate shell. In this case it can be analitically shown (e.g., see Ref.[6]) that the BCS approximation for the isovector pairing does not predict for the binding energy a linear term in $T_z = |N - Z|/2$, specific to the Wigner energy. On the other hand, in the exact solution a linear term in isospin appears naturally through the dependence of energy on $T(T+1)$, which reflects the isospin invariance of the isovector pairing interaction.

There is also a more general argument which indicates that the BCS-like models do not describe properly the isovector proton-neutron pairing correlations in nuclei. Thus, the BCS equations for the isovector pairing in $N=Z$ nuclei have two degenerate solutions, one corresponding to $\Delta_n = \Delta_p \neq 0$ and $\Delta_{np} = 0$ and the other to $\Delta_n = \Delta_p = 0$ and $\Delta_{np} \neq 0$ [7, 8]. This means that in the BCS approximation the isovector proton-neutron pairing does not coexist with the like-particle pairing, as one would expect from the isospin symmetry. Moreover, as shown in Ref.[7], BCS predicts no isovector proton-neutron pairing correlations in the ground state of $N > Z$ nuclei with $T = |T_z|$. One reason why BCS fails to describe properly the isovector proton-neutron correlations is because it does not conserve exactly the particle number and the isospin. The two symmetries can be exactly restored performing projected-BCS (PBCS) calculations. However, the comparison with exactly solvable models shows that PBCS is still unable to provide accurate results for the

isovector pairing correlations [9, 10], which demonstrates the need of going beyond the BCS-type models. In Refs.[10, 11] it was proved that an approach based on quartets formed by two neutrons and two protons coupled to the total isospin $T=0$ can describe with very high accuracy the isovector pairing correlations in the ground state of both $N=Z$ and $N > Z$ nuclei. In this paper we show how this approach can be applied for treating accurately the isovector pairing in self-consistent Hartree-Fock (HF) mean field models. Then, within this framework, we analyse the contribution of the isovector proton-neutron pairing to the symmetry and Wigner energies.

For consistency reason we start by presenting briefly the quartet model introduced in Refs.[10, 11]. This model describes the ground state of a system formed by N neutrons and Z protons moving outside a self-conjugate core and interacting via an isovector pairing force. The Hamiltonian describing this system is

$$\hat{H} = \sum_{i,\tau=\pm 1/2} \varepsilon_{i\tau} N_{i\tau} - g \sum_{i,j,t=-1,0,1} P_{i,t}^+ P_{j,t}, \quad (1)$$

where $\varepsilon_{i\tau}$ are the single-particle energies associated to the mean fields of neutrons ($\tau = 1/2$) and protons ($\tau = -1/2$), supposed invariant to time reversal. The isovector interaction is expressed in terms of the isovector pair operators $P_{i,1}^+ = \nu_i^+ \nu_{\bar{i}}^+$, $P_{i,-1}^+ = \pi_i^+ \pi_{\bar{i}}^+$ and $P_{i,0}^+ = (\nu_i^+ \pi_{\bar{i}}^+ + \pi_i^+ \nu_{\bar{i}}^+)/\sqrt{2}$; the operators ν_i^+ and π_i^+ create, respectively, a neutron and a proton in the state i while \bar{i} denotes the time conjugate of the state i .

Following Ref.[10], the ground state of Hamiltonian (1) for a system with $N=Z$ is described by the state

$$|\Psi\rangle = (A^+)^{n_q} |0\rangle, \quad (2)$$

where $n_q = (N + Z)/4$ and A^+ is the collective quartet built by two isovector pairs coupled to the total isospin $T=0$ defined by

$$A^+ = \sum_{i,j} \bar{x}_{ij} [P_i^+ P_j^+]^{T=0} = \sum_{ij} x_{ij} (P_{i,1}^+ P_{j,-1}^+ + P_{i,-1}^+ P_{j,1}^+ - P_{i,0}^+ P_{j,0}^+). \quad (3)$$

Supposing that the amplitudes x_{ij} are separable, i.e., $x_{ij} = x_i x_j$, the collective quartet operator can be written as

$$A^+ = 2\Gamma_1^+ \Gamma_{-1}^+ - (\Gamma_0^+)^2, \quad (4)$$

where $\Gamma_t^+ = \sum_i x_i P_{i,t}^+$ denote, for $t=0,1,-1$, the collective Cooper pair operators for the proton-neutron (pn), neutron-neutron (nn) and proton-proton (pp) pairs. Thus, in this

approximation the state (2) can be written as

$$|\Psi\rangle = (2\Gamma_1^+\Gamma_{-1}^+ - \Gamma_0^{+2})^{n_q}|0\rangle = \sum_k \binom{n_q}{k} (-1)^{n_q-k} 2^k (\Gamma_1^+\Gamma_{-1}^+)^k \Gamma_0^{+2(n_q-k)}|0\rangle. \quad (5)$$

From the equation above it can be seen that the quartet condensate is a particular superposition of condensates of nn, pp and pn pairs.

In Ref.[11] the quartet condensate model was extended to nuclei with $N > Z$. For these nuclei it is supposed that the neutrons in excess form a pair condensate which is appended to the quartet condensate. Thus, the ground state of $N > Z$ nuclei is approximated by

$$|\Psi\rangle = (\tilde{\Gamma}_1^+)^{n_N} (A^+)^{n_q}|0\rangle = (\tilde{\Gamma}_1^+)^{n_N} (2\Gamma_1^+\Gamma_{-1}^+ - \Gamma_0^{+2})^{n_q}|0\rangle, \quad (6)$$

where $n_N = (N - Z)/2$ is the number of neutron pairs in excess and $n_q = (N - 2n_N + Z)/4$ is the maximum number of alpha-like quartets which can be formed by the neutrons and protons. Since the quartets A^+ have zero isospin, the state (6) has a well-defined total isospin given by the excess neutrons, i.e., $T=n_N$. The neutron pairs in excess are described by the collective pair operator $\tilde{\Gamma}_1^+ = \sum_i y_i P_{i1}^+$, which has a different structure from the collective neutron pair entering in the collective quartet. The mixing amplitudes x_i and y_i which define the ground state (6) are determined from the minimization of $\langle\Psi|H|\Psi\rangle$ under the normalization condition $\langle\Psi|\Psi\rangle = 1$. To calculate the average of the Hamiltonian and the norm it is used the recurrence relations method [10, 11].

In Refs.[10, 11] it was shown that the quartet condensation model (QCM) presented above can describe with very high accuracy (errors below 1%) the pairing correlations induced by the isovector pairing force acting on a given single-particle spectrum. This fact recommends QCM as a proper tool for treating the isovector pairing correlations in self-consistent HF calculations. The calculation scheme we introduce here is similar to the one commonly used in the HF+BCS calculations. Thus, the isovector pairing force is employed as a residual interaction acting on the HF single-particle states from the vicinity of Fermi level. In this study the HF mean field is generated with a zero range Skyrme functional and the HF calculations are performed in a single-particle basis generated by an axially deformed harmonic oscillator, as described in Ref.[12]. After the HF calculations are converged, we select a set of neutron and proton single-particle states with the energies located around the HF chemical potentials. The energies of these states are considered in the Hamiltonian

(1) for performing the QCM calculations. Then, from the QCM calculations we extract the occupation probabilities of the pairing active orbits which are further used to redefine the HF densities. For example, the particle density for neutrons and protons ($\tau = n, p$) are defined by

$$\rho_\tau(r, z) = \sum_i v_{\tau,i}^2 \|\psi_{\tau,i}(r, z)\|^2, \quad (7)$$

where $v_{\tau,i}^2$ are the occupation probabilities for the single-particle states $\psi_{\tau,i}(r, z)$. They are taken equal to 1 (0) for the occupied (unoccupied) HF states which are not considered active in pairing calculations and equal to the QCM values otherwise. The HF and QCM calculations are iterated together until the convergence. Finally, the pairing energy is calculated by averaging the isovector pairing force on the QCM state and is added to the mean-field energy.

As an illustration, the HF+QCM calculation scheme outlined above is applied here for studying the influence of isovector pairing correlations on symmetry and Wigner energies. In the phenomenological mass formulas these energies are parametrized by a quartic and, respectively, a linear term in $N - Z$. Thus, for an isobaric chain with $A=N+Z$ the ground state energy relative to the nucleus with $N=Z$ can be written as

$$E(N, Z) = E(N = Z) + a_A \frac{|N - Z|^2}{A} + a_W \frac{|N - Z|}{A} + \delta E_{shell}(N, Z) + \delta E_P(N, Z). \quad (8)$$

In the equation above it is not considered the contribution of the Coulomb energy, which is supposed to be extracted from all the isotopes of the isobaric chain, and it is also implicitly assumed that for all nuclei with $A=N+Z$ the volume and the surface energies are the same and therefore included in the term $E(N=Z)$. The last two terms in Eq.(8) are the corrections associated to the shell structure and pairing measured relative to the nucleus with $N=Z$. Supposing that these two energy corrections can be also described by a linear and a quartic term in $|N - Z|$ and taking $T = |T_z|$, which is the case for the ground state of nuclei with $A > 40$, Eq.(8) can be written as

$$E(T) = E(T = 0) + \frac{T(T + X)}{2\Phi}, \quad (9)$$

where we have used the notations of Ref.[4]. In the equation above, associated sometimes with the concept of isorotational band [13], X quantifies the contribution of the linear term in isospin to the ground state energy and takes into account all the possible effects, including the ones from the shell structure. The fit of Eq.(8) with experimental data shows that for

many nuclei $a_A \approx a_W$. Thus, when the contribution of the last two terms of Eq.(8) are negligible, $X \approx 1$. In this case the ground state energies of the isobaric chain relative to the nucleus with $N=Z$ depend on $T(T+1)$, as the eigenvalues of the total isospin T^2 . However, a systematic survey based on experimental masses fitted with Eq.(9) [4] shows that X is fluctuating quite strongly around $X = 1$ (see Fig.3 below).

In what follows we analyze the prediction of the HF+QCM calculations for the quantities Φ and X of Eq.(9). The HF+QCM calculations are performed for isobaric chains of even-even nuclei with $A > 40$ for which the ground state has $T = |T_z|$, as supposed in Eq.(9). For each isobaric chain the values of Φ and X are extracted from the binding energies of three nuclei with $T = |T_z| = 0, 2, 4$, i.e., nuclei with $N-Z=0,4,8$. The Skyrme-HF calculations are done with the Skyrme functional SLy4 [14] and neglecting the contribution of the Coulomb interaction. The deformation is calculated self-consistently in axial symmetry using an harmonic oscillator basis [12]. From the HF spectrum we considered in the QCM calculations 10 single-particles states, both for protons and neutrons, above a self-conjugate core. More precisely, for an isobaric chain of mass A , with $A/2$ even, we chose a core with $N_c = Z_c = A/2 - 6$. For the $N=Z$ nucleus this choice corresponds to the QCM state (5) with three quartets, i.e., $n_q = 3$. The same core is kept for calculating the other two isobars with $T=2,4$. They are described by the QCM state (6) with $n_q = 2, n_N = 2$ and, respectively, $n_q = 1, n_N = 4$.

In the HF+QCM calculations one needs a prescription for fixing the strength of the isovector pairing force. According to Refs.[15, 16] the intensity of $T=1$ pairing can be measured by the difference in binding energies between the $T=0$ states in even-even and odd-odd $N=Z$ nuclei. This difference of binding energies is written as

$$2\Delta(N, Z) = \frac{B(N-1, Z-1) - 2B(N, Z) + B(N+1, Z+1)}{2}, \quad (10)$$

where $N=Z=\text{odd}$. For odd-odd $N=Z$ nuclei with $A > 40$ the $T=0$ states one needs to employ in Eq.(10) are excited states. The energies of these states are evaluated by adding to the neighboring even-even $N=Z$ nuclei a neutron and a proton in the single-particle orbits just above the Fermi level and blocking them in the QCM calculations. In Fig.1 are shown the experimental 2Δ , extracted from Ref.[4], in comparison with the HF+QCM results obtained with a state independent isovector force of strength $g = 9.6/A^{3/4}[\text{MeV}]$. One can see that this pairing force gives a reasonable overall agreement with experimental data. Most likely

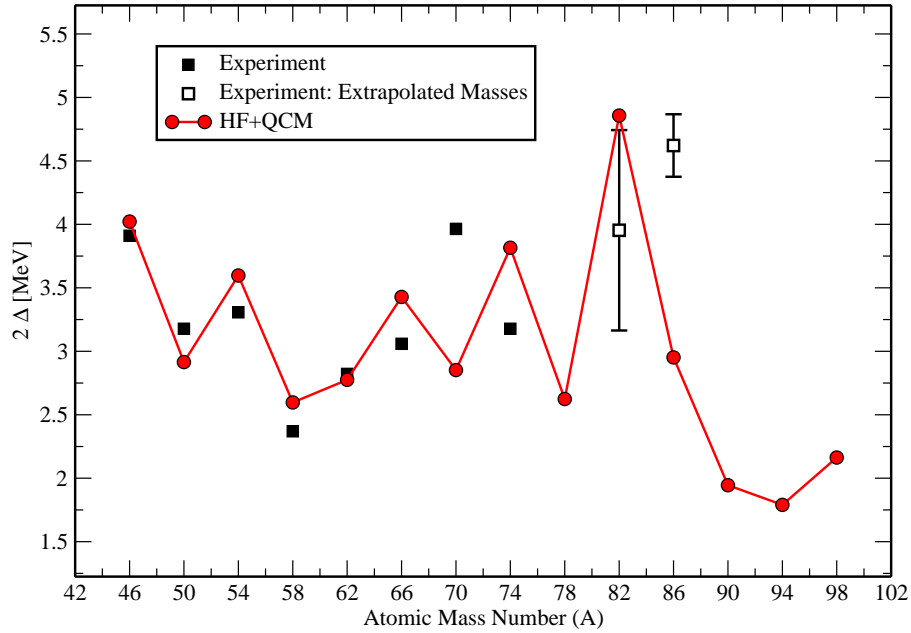


FIG. 1: Even-even to odd-odd mass difference along the $N=Z$ line calculated by Eq.(10) as a function of mass number. The experimental values, including the ones calculated from extrapolated masses, are from Ref.[4].

the largest deviations seen in Fig.1 are related to the crude approximation employed to calculate the excited $T=0$ states (e.g., the effect of the $T=0$ interaction is neglected) and to the inaccuracy of HF level densities around the Fermi levels (see below).

Figs.2-3 display the results of HF+QCM calculations for $1/\Phi$ and X in comparison with the experimental values [4]. The latter are obtained employing in Eq.(9) the experimental masses of Ref.[17] from which the Coulomb energy was removed (for details, see [4]). In these figures are shown also the results of HF+BCS calculations. In the BCS calculations, performed with the same model space and cores as in the QCM calculations, the pairing correlations for protons and neutrons are treated independently and the proton-neutron pairing is not taken into account.

From Fig.2 one can notice that the HF+QCM calculations describe very well the mass dependence of the quantity $1/\Phi$ associated to the standard symmetry energy proportional

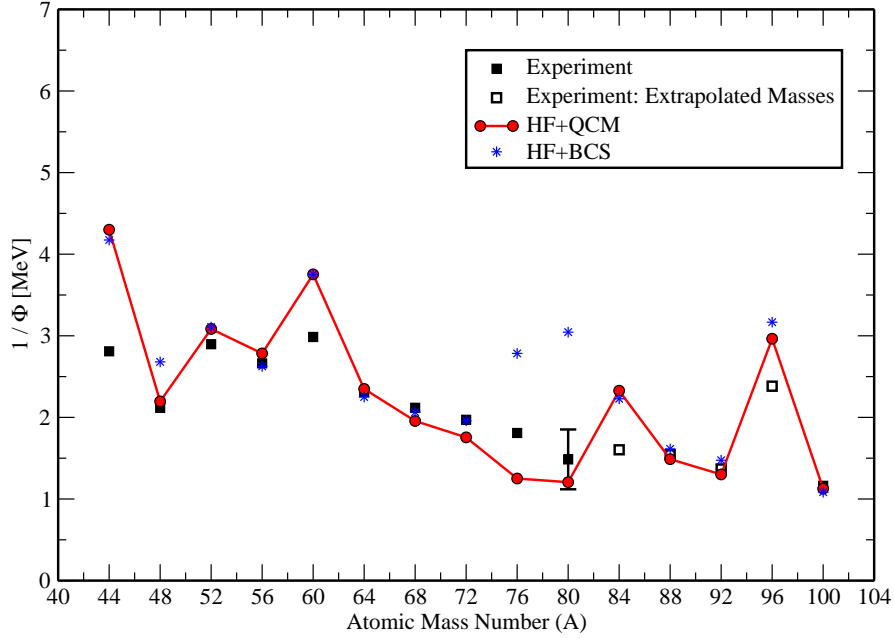


FIG. 2: The quantity $1/\Phi$ (see Eq.(9)), expressing the strength of the symmetry energy term proportional to T^2 , as a function of mass number. The experimental values, obtained by removing the contribution of Coulomb energy, are from Ref.[4].

to T^2 . The largest deviations appear for the isotopic chains which cross a magic number at $T=2$, i.e., for the nuclei with $N-Z=4$. The discrepancies are related to the inaccuracy of the deformations predicted by the mean field calculations for nuclei with two particles or two holes above/below a magic or semi-magic number. As an example we discuss here the result for the chain $A=44$ which shows the largest deviation from the experiment. The HF+QCM calculations predict almost zero deformation for ^{44}Ti and ^{44}Cr and a deformation of $\beta_2 = 0.19$ for ^{44}Ar . The experimental deformations for these isotopes are, respectively, $\beta_2 = 0.268, 0.253, 0.240$ [18]. Thus, contrary to what the experimental deformations indicate, in the calculations there is a large energy gap between the shells $f_{7/2}$ and $d_{3/2}$ which means that the energy difference $E(T=4)-E(T=2)$ is overestimated. On the other hand, the energy difference $E(T=2)-E(T=0)$ is underestimated since in going from $T=0$ to $T=2$ the pairs are interchanged within the degenerate $f_{7/2}$ shell. Consequently, because $1/\Phi = E(T =$

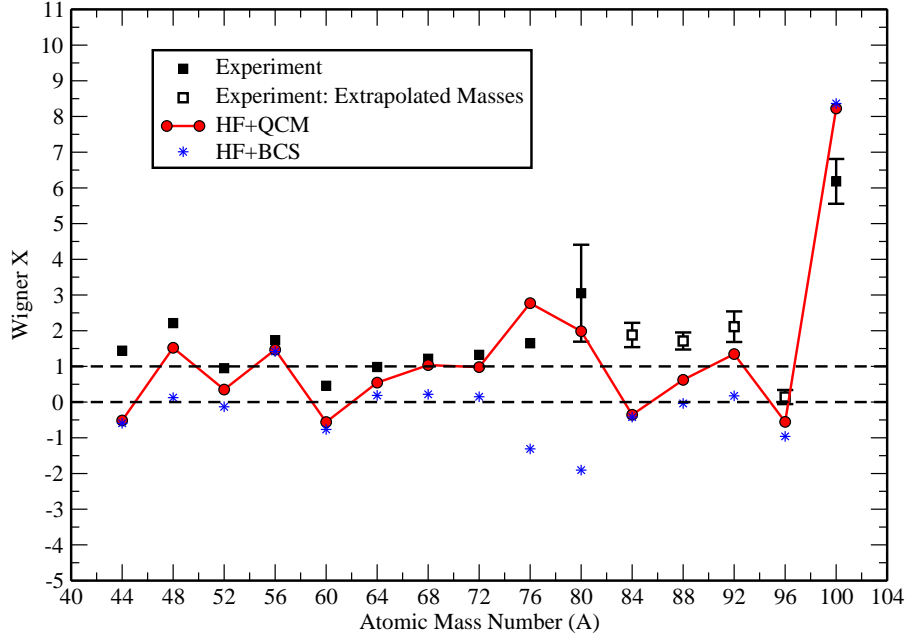


FIG. 3: The quantity X (see Eq.(9)), which gives the contribution of Wigner energy relative to the standard symmetry energy, as a function of mass number. The experimental values, obtained by removing the contribution of Coulomb energy, are from Ref.[4].

4) $-E(T=2) - [E(T=2) - E(T=0)]$, the calculated value of $1/\Phi$ for $A=44$ is largely overestimated compared to the experiment. A similar mechanism applies for the chains $A = 60, 84, 96$. From Fig.2 we can also observe that HF+BCS and HF+QCM give quite similar results for $1/\Phi$, suggesting that the isovector proton-neutron pairing does not play a major role for the standard symmetry energy.

The predictions for the quantity X are shown in Fig.3. One can now notice that the HF+BCS calculations fail to describe the linear term in T associated to Wigner energy (see also Ref.[19]). In fact, as seen in Fig.3, for the majority of chains the HF+BCS calculations predict for X values close to zero. On the other hand we observe that the HF+QCM results are following well the large fluctuations of X with the mass number. The largest deviations from experimental values appear again for the isobaric chains which cross a magic number for $T=2$. It can be thus seen that for these chains the calculated X values are underes-

timated (overestimated) when $1/\Phi$ are overestimated (underestimated). This fact can be simply traced back to the expression $X=(3r-1)/(r-1)$, where $r=(E(4)-E(2))/(E(2)-E(0))$. For example, the underestimation of X for the chain $A=44$ is due to the overestimation of the ratio r , which reflects the overestimation of $1/\Phi$ discussed above. Thus, as in the case of $1/\Phi$, the largest discrepancies of X seen in Fig.3 are related to the inaccuracy of level densities predicted by mean field model for nuclei with two neutron or two holes above/below a magic number.

A similar effect of the shell fluctuations on Wigner energy was noticed earlier [4] by using a different calculation scheme based on an isovector pairing force, diagonalized in a restricted model space, and a phenomenological T^2 interaction introduced to simulate the isospin dependence of the single-particle levels. It is remarkably to observe that the HF+QCM calculations, in which the isospin dependence of the single-particle is consistently taken into account, give very good results for the symmetry and Wigner energy terms, comparable in accuracy with the results of Refs.[4, 5] obtained with additional fitting parameters.

In conclusion, in this paper we have shown how the isovector pairing interaction can be treated in the mean-field models by conserving exactly the particle number and the isospin. To treat the isovector pairing correlations we use a condensate of alpha-type quartets to which it is appended, in the case of nuclei with $N > Z$, a condensate of neutron pairs. This formalism is applied to analyse the effect of isovector pairing on symmetry and Wigner energies. The results show that the isovector pairing acting on a self-consistent mean field can explain reasonably well the mass dependence of Wigner energy. In principle, the latter can be also influenced by the isoscalar proton-neutron pairing. This issue will be addressed in a future publication.

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